# $\chi^2$ AND POISSONIAN DATA: BIASES EVEN IN THE HIGH-COUNT REGIME AND HOW TO AVOID THEM

Philip J. Humphrey<sup>1</sup>, Wenhao Liu<sup>1</sup> & David A. Buote<sup>1</sup>

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# ABSTRACT

We demonstrate that two approximations to the  $\chi^2$  statistic as popularly employed by observational astronomers for fitting Poisson-distributed data can give rise to intrinsically biased model parameter estimates, even in the high counts regime, unless care is taken over the parameterization of the problem. For a small number of problems, previous studies have shown that the fractional bias introduced by these approximations is often small when the counts are high. However, we show that for a broad class of problem, unless the number of data bins is far smaller than  $\sqrt{N_c}$ , where  $N_c$  is the total number of counts in the dataset, the bias will still likely be comparable to, or even exceed, the statistical error. Conversely, we find that fits using Cash's C-statistic give comparatively unbiased parameter estimates when the counts are high. Taking into account their well-known problems in the low count regime, we conclude that these approximate  $\chi^2$  methods should not routinely be used for fitting an arbitrary, parameterized model to Poisson-distributed data, irrespective of the number of counts per bin, and instead the C-statistic should be adopted. We discuss several practical aspects of using the C-statistic in modelling real data. We illustrate the bias for two specific problems— measuring the count-rate from a lightcurve and obtaining the temperature of a thermal plasma from its X-ray spectrum measured with the Chandra X-ray observatory. In the context of X-ray astronomy, we argue the bias could give rise to systematically mis-calibrated satellites and a  $\sim 5-10\%$  shift in galaxy cluster scaling relations.

### 1. INTRODUCTION

When faced with the problem of fitting a parameterized model to Poisson-distributed data, observational astronomers typically adopt one of two approaches. First, the maximum likelihood method involves varying the model parameters until the probability density function of the data given the model is maximal. In practice, observers typically minimize a statistic such as C, defined by Cash (1979) which, in a slightly modified form (as implemented in the astronomical X-ray spectral-fitting package *Xspec*; Arnaud 1996), can be written

$$C = 2\sum_{i} M_i - D_i + D_i \log D_i - D_i \log M_i \qquad (1)$$

where  $D_i$  is the number of detected counts in the i<sup>th</sup> data-bin,  $M_i \equiv M_i(p_1, \ldots, p_k)$  is the model being fitted, and  $p_1, \ldots, p_k$  are the model parameters.

Since the absolute value of the C-statistic cannot be directly interpreted as a goodness-of-fit indicator, observers typically prefer instead to minimize the better-known  $\chi^2$  fit statistic (e.g. Lampton et al. 1976). As that statistic is strictly only defined for Gaussian-distributed data, observers generally approximate the true  $\chi^2$  by a data-based summation of the form

$$\chi^2 \simeq \chi_d^2 = \sum_i \frac{(M_i - D_i)^2}{D_i} \tag{2}$$

or

$$\chi^2 \simeq \chi_m^2 = \sum_i \frac{(M_i - D_i)^2}{M_i}$$
 (3)

where the d and m subscripts indicate whether the data or the model are used as weights. In the literature these two weighting choices are sometimes referred to as "Neyman's" and "Pearson's", respectively. The shortcomings of these approximations are well-documented when there are few counts per bin. Cash (1979) pointed out that deviations from Gaussianity make such approximations inaccurate when the counts per bin fall below  $\sim 10-20$ , and various authors have quantified how the best-fitting parameters obtained from minimizing  $\chi_m^2$  and  $\chi_d^2$  for specific models become biased below this limit (e.g. Nousek & Shue 1989; Wheaton et al. 1995; Churazov et al. 1996; Leccardi & Molendi 2007). A number of other approximations to  $\chi^2$  have been proposed to mitigate this effect (e.g. Wheaton et al. 1995; Kearns et al. 1995; Churazov et al. 1996; Mighell 1999). In contrast, at least for some problems, fits using the C-statistic are found to be far less biased for low counts data (e.g. Nousek & Shue 1989; Churazov et al. 1996; Arzner et al. 2007), although not completely so (Leccardi & Molendi 2007).

When the number of counts per bin exceeds  $\sim 15-20$ , the deviations from Gaussianity become less severe. Therefore, it is common practice in observational astronomy to assume that, in such cases,  $\chi^2_d$  and  $\chi^2_m$  sufficiently well approximate the true  $\chi^2$  and that the model parameters for an arbitrarily parameterized model that minimize those statistics are relatively unbiased estimates of the true parameter values. The meaning of "relatively" here depends on context; for most observers a non-negligible bias would be acceptable provided it does not lead to the wrong scientific conclusions. This pragmatic approach to statistical inference is common in the observational literature, but differs from the more rigorous methods gen-

<sup>&</sup>lt;sup>1</sup> Department of Physics and Astronomy, University of California, Irvine, 4129 Frederick Reines Hall, Irvine, CA 92697-4575

erally preferred among statisticians. Nevertheless, when employing any approximation, it should be contingent upon the observer to assess whether it could potentially lead to wrong conclusions. Unfortunately, this is seldom done, and approximations such as  $\chi^2_d$  or  $\chi^2_m$  are often used without comment for a given problem.

For the simple problem of measuring the count-rate of a (non-varying) source given its lightcurve, a number of authors have assessed the accuracy of using the  $\chi_d^2$  and  $\chi_m^2$  approximations. As the count-rate becomes large, the fitted count-rate which minimizes  $\chi_d^2$  is asymptotically found to underestimate the true rate by  $\sim \tau^{-1}$  count s<sup>-1</sup>, while similar fits using  $\chi_m^2$  overestimate it by  $\sim 0.5\tau^{-1}$  count s<sup>-1</sup>, where  $\tau$  is the duration (in seconds) of each bin (Wheaton et al. 1995; Jading & Riisager 1996; Mighell 1999; Hauschild & Jentschel 2001). This can be understood as arising from the misparameterization of the problem; when one puts  $M_i = p\tau$ , where p is the count-rate of the source, the dependence of the denominator in Eqn 3 on p naturally leads to a bias. Similarly, the dependence of the denominator in Eqn 2 on the observed data also produces a systematic bias when minimizing  $\chi_d^2$  with respect to p (Wheaton et al. 1995; Jading & Riisager 1996). Nonetheless, as the number of counts increases this corresponds to an increasingly small fractional bias. If one only requires to know the absolute count-rate to a given fractional accuracy, therefore, the use of  $\chi_d^2$  or  $\chi_m^2$  may be "good enough", provided the count rate is sufficiently high.

In this paper, we point out that a more relevant quantity than the fractional bias for assessing the usefulness of the approximations used in fitting is  $f_b$ , the bias divided by the statistical error. For two very different physical problems, obtaining the count-rate from a lightcurve and obtaining the temperature of a thermal plasma from its X-ray spectrum, we compute  $f_b$  for fits to realistic data which minimize  $\chi_d^2$ ,  $\chi_m^2$  and C. For  $\chi_d^2$  and  $\chi_m^2$  fits, we find that  $f_b$  can be of order unity, or even worse, even if the number of photons per bin far exceeds the nominal  $\sim 20$  counts. In contrast, for the C-statistic fits, we find  $|f_b| \ll 1$ . We explain these results in terms of an approximate, analytical expression for  $f_b$  for each statistic, and show that fits of an arbitrary, parameterized model are, in general, far less biased when the C-statistic is employed than  $\chi^2_d$  or  $\chi^2_m$ , unless the model parameterization is chosen carefully. Finally, we discuss the possible scientific impact of the bias, as well as the advantages and practical implementation of using the C-statistic instead for data-modelling. We stress that we are not, in this paper, attempting a formal, statistical assessment of the validity of using  $\chi^2$  methods in general to model any particular problem, but rather we are asking whether the current approximate  $\chi^2$  methods for Poisson-distributed data that are widely employed by observers are useful (in the sense  $|f_b| \ll 1$ ).

### 2. THE BIAS

In this section, we investigate two very different problems, specifically the linear problem of obtaining the count-rate of a (non-variable) source from its lightcurve and the highly nonlinear problem of obtaining the temperature of a thermal plasma from its X-ray spectrum. We use Monte Carlo simulations to measure  $f_b$  as a function of the "true" parameter value, the number of counts

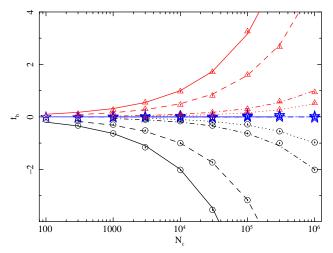


FIG. 1.—  $f_b$  for the lightcurve model, as a function of total counts  $N_c$  in the lightcurve. Circles denote  $f_b$  obtained with the  $\chi^2_d$  statistic, triangles are for  $\chi^2_m$  fits, and stars are for C-statistic minimization. Results are shown for 50, 100, 500 and 1000 counts per bin (solid lines, dashed lines, dot-dash lines and dotted lines, respectively). The lines are the analytical approximations discussed in § 3.

in each dataset and the adopted binning.

### 2.1. Lightcurve

We first considered the problem  $M_{i0} = p_0 \tau$ , where  $M_{i0}$ is the true model value in the i<sup>th</sup> bin,  $\tau$  is the binsize of the lightcurve and  $p_0$  the true count-rate of the source. We sought an estimate of  $p_0$  by fitting a model of the form  $M_i = p\tau$  to the data. For each of a range of different values of  $p_0$  (50, 100, 500 and 1000 count s<sup>-1</sup>) and  $N_c$ , we simulated a set of 1000 lightcurves with  $\tau = 1$  s, assuming that the total counts per bin were Poisson distributed about  $p_0\tau$ . For each simulated lightcurve we used customized software built around the MINUIT software library<sup>2</sup> to obtain the value of p which minimized each statistic  $(\chi_d^2, \chi_m^2)$  and C). The mean and standard deviation of the best-fitting p values were measured for each  $(p_0, N_c)$  pair and statistic choice, allowing  $f_b$  to be computed. In Fig 1, we show how  $f_b$  varies as a function of  $N_c$ , the total counts in the lightcurve, and the count-rate of the source.

As is clear from Fig 1, at fixed count-rate and binsize, the statistical importance of the  $\chi^2_d$  and  $\chi^2_m$  bias is an increasing function of the number of counts in the lightcurve; indeed it rapidly becomes very large as the number of data-bins gets large. This is simply because the absolute value of the bias is approximately constant as the count-rate becomes large (Jading & Riisager 1996), whereas the statistical error is a decreasing function of  $N_c$ . In stark contrast, for the Cash C-statistic fits, we find  $|f_b| \ll 1$ ; in fact the bias using the C-statistic is exactly zero here. This can be seen by substituting  $M_i = p\tau$  into Eqn 1 and analytically minimizing C, which leads to  $p = \sum_i D_i / \sum_i \tau$ , the expectation of which is  $p_0$ .

## $2.2. \ Thermal\ plasma$

We next consider the case of an X-ray emitting, optically thin, collisionally ionized thermal astrophysical

 $^2 \\ http://lcgapp.cern.ch/project/cls/work-packages/mathlibs/minuit/index.html$ 

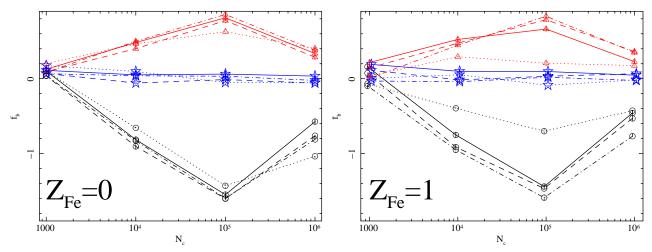


Fig. 2.—  $f_b$  for the recovered temperature of a thermal plasma from its Chandra X-ray spectrum, as a function of total counts  $N_c$  in the spectrum, for a thermal plasma with zero metal abundance ( $Z_{Fe}=0$ ) and for a Solar abundance plasma ( $Z_{Fe}=1$ ). The data-points represent the results of the Monte Carlo simulations (see text), and the error-bars on  $f_b$  are all  $\sim 0.03$ . Circles denote  $f_b$  for the  $\chi_d^2$  fits, triangles indicate  $\chi_m^2$  fits, and stars indicate C-statistic minimization. The temperature of the thermal plasma is indicated by the style of the line joining the data-points, with solid, dashed, dot-dash and dotted lines indicating a plasma with kT=1, 3, 5 and 7 keV, respectively.

plasma, the X-ray spectrum of which is dominated by thermal bremsstrahlung plus line emission. Using the Xspec spectral-fitting package we simulated and fitted spectra which might be observed with the ACIS-I instrument aboard the Chandra X-ray observatory. Since we considered the high count limit, we did not include any background in the simulations. For the source model we used a zero redshift APEC (Smith et al. 2001) plasma model modified by line-of-sight absorption due to the cold Galactic ISM (Bałucińska-Church & McCammon 1992). We assumed an absorption hydrogen columndensity of  $10^{20} cm^{-2}$ , consistent with a high Galactic latitude pointing. The redistribution matrix (RMF) and effective area (ARF) files (which map the physical source model onto the binned data taken by the detector) were created for a near-aimpoint position in a representative ACIS-I observation.

Using the "fakeit" command in Xspec we simulated sets of 1000 spectra for different combinations of temperature, metal abundance and total counts per spectrum. This procedure creates data in a set of pre-defined bins by drawing a random number from a Poisson distribution with intrinsic mean  $M_{i0}$ , i.e. the expected counts predicted by the model. We have verified that we obtain consistent results with our own software. We chose input temperatures of 1, 3, 5 and 7 keV/k respectively and each model has heavy element abundances relative to hydrogen set either to zero, or to match the Solar values (Grevesse & Sauval 1998). We considered data only in the 0.5–7.0 keV range, and simulated spectra with a range of  $N_c$  spanning  $10^3$  to  $10^6$ , In each spectrum, the simulated data points were regrouped to ensure at least 20 photons per bin. We fitted each simulated spectrum while allowing only the temperature and normalization to vary, separately using  $\chi_d^2$ ,  $\chi_m^2$  and the C-statistic, all of which are implemented as standard in Xspec. We show  $f_b$  obtained with each statistic as a function of temperature, heavy element abundance and  $N_c$  in Fig 2. In contrast to the  $\chi_d^2$  and  $\chi_m^2$  fits, for which  $|f_b| \sim 0.5$ –1 it is immediately apparent that the C-statistic results are practially unbiased.

#### 3. DISCUSSION

For the two very different problems discussed in § 2, we find that, using realistic data,  $|f_b| \ll 1$  only for the fits using the C-statistic while the best-fitting parameters obtained by minimizing  $\chi_d^2$  and  $\chi_m^2$  were significantly biased ( $f_b$  of order unity). In order to explain these results, in the Appendices we derive an approximate analytical expression for the order of magnitude of  $f_b$  given an arbitrarily parameterized model. For fits using  $\chi_d^2$ , we find  $f_b \sim \mp N/\sqrt{N_c}$ , where N is the number of data-bins and  $N_c$  the number of counts in the data-set. Alternatively, fits using  $\chi_m^2$  were biased in the opposite sense, yielding  $f_b \sim \pm 0.5 N/\sqrt{N_c}$ . This is true even in cases where the number of counts far exceeds the canonical 20 per bin required for deviations from Gaussianity to be unimportant. As pointed out by Wheaton et al. (1995), the bias arises not from deviations from Gaussianity but because of the misparameterization of the problem when these approximations are used with an arbitrary model. In contrast, those fits employing the C-statistic typically should have  $|f_b| \ll 1$ . We show these order of magnitude estimates for the lightcurve problem as the various lines in Fig 1, revealing excellent agreement with the results of our simulations<sup>3</sup>.

The values of  $f_b$  obtained for the spectral-fitting problem (Fig 2) are also easily understood in terms of these order of magnitude estimates. In the regime of relatively few counts ( $\sim 1000$  per spectrum), the statistical errors can be quite large (e.g.  $\pm 3$  keV for the 7 keV plasma) and hence  $f_b$  was small for all the statistics. For the cases with more counts the error-bars were small enough that the truncated Taylor expansion used in the Appendices is approximately valid. Considering a typical 7 keV plasma with  $N_c=10^5$ , N is  $\sim 400$ , implying  $f_b \sim -1.3$  for  $\chi_d^2$  fits, which is close to the observed value. As  $N_c$  falls, so too does N since more data-bins need to be grouped together to ensure at least 20 counts in each. This can more than offset the fall in  $N_c$  and prevents  $f_b$  from growing much

<sup>&</sup>lt;sup>3</sup> In fact, for this problem, these estimates are almost exact, as can be seen by substituing the  $M_i=p\tau$  into the derivations in the appendices.

larger. In contrast, as  $N_c$  gets even larger, there are few bins at the original instrument resolution which contain fewer than 20 counts (i.e. that need to be regrouped) and so N grows only slightly from  $10^5$  to  $10^6$  counts. Thus  $f_b$  starts to fall as  $N_c$  gets very large, as seen in Fig 2. A similar argument explains the trend of  $f_b$  with  $N_c$  for the  $\chi^2_m$  fits.

### 3.1. Removing the bias

We have shown that, for fitting Poisson-distributed data with an arbitrary, parameterized model even in a fairly high-counts regime, the routine use of the  $\chi^2_d$  and  $\chi^2_m$  approximations to the true  $\chi^2$  is likely to give rise to biases in the best-fitting parameters which can be of order the statistical error, or even larger. We argue, therefore, that the  $\chi^2_d$  and  $\chi^2_m$  approximations should generally be avoided for fitting Poisson-distributed data, unless the square root of the number of counts in the dataset far exceeds the number of bins being fitted, or the model parameterization is chosen with care. In contrast, fits performed using the Cash C-statistic yield estimates which are, to all practical purposes, unbiased in the regimes we have discussed in this paper and we, therefore, strongly recommend its use instead.

The major objection to the widespread uptake of the C-statistic for model-fitting is that the statistic itself cannot be directly interpreted as a goodness-of-fit indicator in a similar fashion to the (true)  $\chi^2$  statistic. In order to test the hypothesis that the data are consistent with the (best-fitting) model, therefore one must adopt an alternative strategy. Arguably the most robust technique<sup>4</sup> is a fairly costly Monte Carlo approach, for example that implemented as the "goodness" command in Xspec. On each simulation, an artificial dataset is generated by adding Poisson-noise to the best-fitting model, and the artificial data are fitted. The fraction of simulations which yield a best-fitting statistic value which is more negative (i.e. a better fit) than the best-fit statistic for the real data is an estimate of the significance at which the null hypothesis can be rejected. We note that the distribution of the best-fitting parameter values from these simulations can be used at minimal extra computational cost to derive a confidence interval for each parameter (e.g. Humphrey et al. 2006; Buote et al. 2003), as well as providing a direct assessment of the magnitude of any residual bias. In the case where the number of fitted parameters becomes large, this Monte Carlo method of error-bar estimation is far more efficient than the more usual procedure of stepping through parameter space (e.g. Cash 1979).

While it is not strictly necessary to bin the data in order to fit a model with the C-statistic, the choice of binning is critical for interpreting the goodness-of-fit (e.g. Helsdon et al. 2005). The reason is that the statistic is defined only locally, in the sense that it contains no information about the relative ordering of the residuals between data and model. To illustrate this point, consider testing a lightcurve with the model  $M_i = p\tau$ . Let the data be sufficiently sparsely binned that the number of counts in bin i,  $D_i$  can only equal 0 or 1, and further

let all of the nonzero data-points be in the second half of the lightcurve (which clearly has only a  $\sim 2^{-N_c}$  chance of occurring randomly, if the model is correct). Substituting the best-fitting value  $(p=N_c/N\tau)$  into Eqn 1, it is clear that

$$C = 2\sum_{i} D_{i}logD_{i} - 2N_{c}log\left(\frac{N_{c}}{N}\right) = -2N_{c}log\left(\frac{N_{c}}{N}\right)$$

i.e. C depends only on the number of counts in the lightcurve, and not their relative order. On each Monte Carlo simulation we generate an artificial lightcurve from the best-fitting model, so clearly approximately half will have more than  $N_c$  counts in total, and half will have fewer. Provided  $N_c/N \ll \exp(-1)$ , which must be true in this case, C varies monotonically with  $N_c$  and so the estimated null hypothesis probability will be 0.5 (i.e. a "good fit"). Alternatively, one can rebin the data into two equally-sized bins (one containing 0 counts and one  $N_c$ ), in which case the  $\sum_i D_i log D_i$  term is no longer 0 and the test has greater power to distinguish between the model and the data. Based on Monte Carlo simulations, the model will be rejected at better than 99.9% significance provided  $N_c \gtrsim 8$ . It is worth noting, however, that increasing the binning is not always helpful; if we were to bin the data even more heavily (into a single bin), we would wash out the information which allows us to distinguish between the model and the data. In the case that the data are inconsistent with the model, the null hypothesis probability is almost always a strong function of the adopted binning.

It is important to appreciate that the dependence of the null hypothesis probability on the binning of the data is by no means limited to uses of the C-statistic, since  $\chi^2$  (which also contains no information about the grouping of the residuals) suffers from exactly the same problem (Gumbel 1943). In practice, the appropriate binning to use is that which maximizes the difference between the data and the model, which likely depends on the precise model being fitted and may involve some experimentation. Choosing to adopt the  $\chi^2_m$  approximation on the grounds that it is "easily interpretable" for an ad hoc binning scheme is clearly something of a false economy, especially coupled with the intrinsic bias which can arise when it is used. The problem is exacerbated for the  $\chi^2_d$  statistic, which is only approximately  $\chi^2$  distributed (Hauschild & Jentschel 2001).

Our present discussion does not consider the potential impact of background uncertainties (which can introduce additional systematic errors; e.g. Liu et al. 2008), nor the case of very few counts per bin. In these circumstances it is possible that bias may remain on best-fitting parameters recovered from C-statistic fitting, or its variant in the *Xspec* package which takes account of direct background subtraction (Leccardi & Molendi 2007). A full assessment of such putative effects needs to be carried out on a case-by-case basis, but is relatively straightforward with the Monte Carlo method outlined above, and we will address some of these issues in a future paper (Liu et al. 2008).

Alternative approximations to  $\chi^2$  have been proposed which are less biased in the case of very few counts per bin (where the bias is partially due to deviations from Gaussianity). In general these schemes (e.g. Wheaton et al. 1995; Kearns et al. 1995; Churazov et al. 1996)

<sup>&</sup>lt;sup>4</sup> For example, the method outlined by Baker & Cousins (1984) may not be accurate in all count regimes (Hauschild & Jentschel 2001).

are not rigorously motivated and there is no good theoretical reason to expect them to yield genuinely unbiased estimates for any given problem in the high counts case. Coupled with their lack of widespread use and the difficulty of assessing their performance analytically, we do not address them here other than to state that, aside from the ostensible transparency of the  $\chi^2$  value (which, as stated above, can be deceptive), we see little compelling reason to use them in preference to the C-statistic.

# 3.2. Scientific impact of the $\chi^2$ bias

The existence of the bias will undoubtedly have implications for the scientific conclusions of various studies which have adopted  $\chi^2_d$  or  $\chi^2_m$  approximations for fitting Poisson distributed data without assessing the limitations of these approximations in that context. In this section, we highlight a few cases of particular interest from the field of X-ray astronomy, in which  $\chi^2_d$  is typically adopted as a de facto standard (e.g. in Xspec).

The in-flight inter-calibration of X-ray satellites can be assessed by comparing spectral-fits of very bright, canonical "calibration sources" (e.g. Kirsch et al. 2005; Plucinsky et al. 2008). Since different X-ray instruments have different numbers of spectral bins (e.g. typically  $\lesssim 500$ for the XMM PN and typically  $\lesssim 50$  for the RossiXTE PCA) and since differences in exposure time and collecting area mean that there are widely varying numbers of photons in the calibration datasets, the absolute magnitude of the bias is expected to vary from instrument to instrument. For realistic sources it can be of order a few percent or higher, which is competetive with the absolute target calibration of most instruments. Since calibration sources are generally very bright, the statistical errors on recovered parameters are typically very small, and hence we may see parameter spaces which do not overlap even if the satellites are perfectly inter-calibrated.

X-ray studies of galaxy clusters and groups routinely involve the computation of gravitating mass profiles from the measured gas temperature and density profiles (obtained from spatially-resolved spectroscopy) and the equation of hydrostatic equilibrium (e.g. Gastaldello et al. 2007). Based on our simulations, and the arguments in Appendix A, we expect roughly a 5-10% fractional bias on the temperature, which would translate into a similar bias on the mass, especially in the cluster regime. Errors of this magnitude are significant if clusters are to be used for precision cosmology measurements. As an example, the relation between a cluster's virial mass (M<sub>vir</sub>) and dark matter halo concentration (c), both of which are derived by fitting a canonical dark matter halo model (the NFW profile) to the measured mass profile, can be used to distinguish between cosmological models. Clearly M<sub>vir</sub> is likely to be underestimated due to the bias but the effect on c is harder to predict since it depends sensitively on the exact slope of the mass profile, which in turn depends on how the bias varies with radius. Still, if c is systematically biased by as much as  $\sim 5\%$ , as in our example below, that

would be comparable to the current best statistical error on the normalization of the c- $M_{\rm vir}$  relation, which is the prime discriminator between different cosmological models (Buote et al. 2007).

To illustrate the bias on  $M_{vir}$  and c with real data, we have reduced and analysed high-quality Chandra data of a nearby, X-ray bright cluster, A 1991. We obtained 39 ks of data from the *Chandra* archive, which we processed to obtain the temperature, gas density and gravitating mass profiles as outlined in Gastaldello et al. (2007). Using the C-statistic we fitted the data in 9 radial bins with parameterized models for the gas temperature and density which, inserted into the equation of hydrostatic equilibrium, enabled us to obtain the mass profile and hence  $M_{\rm vir}$  and c. We found  $M_{\rm vir} = 2.60 \pm 0.19 \times 10^{13} M_{\odot}$ and c=  $7.94 \pm 0.47$ , which are broadly consistent with the measurements of Vikhlinin et al. (2006), who apparently used  $\chi_d^2$ . Refitting the data, this time using  $\chi_d^2$ , we found that the temperature was reduced by  $\sim 2\%$  on average and in individual bins it could change by as much as  $\sim 1-\sigma$ . This bias translated into a  $\sim 4\%$  reduction in the resulting  $M_{vir}$  and c, or a  $\sim 0.5$ - $\sigma$  effect. The full details of this analysis will be given in Liu et al. (2008).

Another scaling relation which is key for understanding cluster physics is the relation between  $M_{\rm vir}$  and the emission-weighted X-ray temperature of the gas,  $T_{\rm X}$ . Both  $T_{\rm X}$  and  $M_{\rm vir}$  are likely underestimated in most published studies (which generally use  $\chi^2_d$ ). Since the spectrum used to measure the temperature usually contains far more counts than any of the individual spectra used to determine the mass profile, the effect on  $M_{\rm vir}$  is likely to be much larger. If this effect is as large as our estimated  $\sim 5-10\%$ , it will not only exceed the current best statistical error on the normalization of the measured relation, but it will also partially reduce the  $\sim 30\%$  discrepancy in the normalization between the measured relation and the predictions of self-similar models of cluster formation (e.g. Arnaud et al. 2005).

As a final illustration of the effects of the bias in real data analysis, in his X-ray study of the hot gas in galaxy groups, Buote (2000) estimated error-bars on the temperature and Fe abundance by a Monte Carlo procedure similar to that discussed in § 3.1. In a significant number of cases, the 1- $\sigma$  error range inferred from the simulations did not actually contain the best-fitting parameter (i.e. the bias was more than 1- $\sigma$ ), giving rise to error-bars which appeared distorted when plotted.

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### APPENDIX

## A. BIAS IN $\chi^2$ -FITTING

### A1. Data weighting

We here derive an expression for the magnitude of the bias when fitting a parameterized model using the  $\chi_d^2$  approximation. We start by setting  $M_i = M_i(p)$ , with the parameter p having a true value  $p_0$  and defining  $M_{i0} = M_i(p_0)$ . Starting with Eqn 2, differentiating with respect to p and setting the derivative equal to zero, we obtain:

$$0 = \frac{d\chi_d^2}{dp} = 2\sum_i \frac{dM_i}{dp} \left(\frac{M_i - D_i}{D_i}\right) \tag{A1}$$

Now, we write  $D_i = M_{i0} + \delta D_i$  and  $M_i \simeq M_{i0} + \delta p M'_{i0} + \delta p^2 M''_{i0}/2 + \dots$ , where  $M'_{i0} = dM_i/dp$  evaluated at  $p = p_0$ , and so on. Substituting these in and rearranging we obtain:

$$0 = \sum_{i} -\frac{M'_{i0}}{M_{i0}} \delta D_{i} + \sum_{i} \frac{M'_{i0}}{M_{i0}^{2}} \delta D_{i}^{2} + \delta p \left[ \sum_{i} \frac{M'_{i0}}{M_{i0}} + \sum_{i} \left( -\frac{M'_{i0}}{M_{i0}^{2}} - \frac{M''_{i0}}{M_{i0}} \right) \delta D_{i} + \sum_{i} \left( \frac{M'_{i0}}{M_{i0}^{3}} + \frac{M''_{i0}}{M_{i0}^{2}} \right) \delta D_{i}^{2} \right]$$

$$+ \delta p^{2} \left[ \sum_{i} \frac{3M'_{i0}M''_{i0}}{2M_{i0}} + \sum_{i} \left( -\frac{3M'_{i0}M''_{i0}}{2M_{i0}^{2}} - \frac{M'''_{i0}}{2M_{i0}} \right) \delta D_{i} + \sum_{i} \left( \frac{3M'_{i0}M''_{i0}}{2M_{i0}^{3}} + \frac{M'''_{i0}}{2M_{i0}^{2}} \right) \delta D_{i}^{2} \right] + \dots$$

$$(A2)$$

If higher order terms can be ignored, this is just a quadratic equation of the form:

$$0 = \sum_{i} a_{i} \delta D_{i} + \sum_{i} a'_{i} \delta D_{i}^{2} + \delta p \left( B + \sum_{i} b_{i} \delta D_{i} + \sum_{i} b'_{i} \delta D_{i}^{2} \right) +$$

$$\delta p^{2} \left( C + \sum_{i} c_{i} \delta D_{i} + \sum_{i} c'_{i} \delta D_{i}^{2} \right)$$

$$\Rightarrow \delta p = \frac{-(B + \sum_{i} b_{i} \delta D_{i} + \sum_{i} b'_{i} \delta D_{i}^{2})}{2(C + \sum_{i} c_{i} \delta D_{i} + \sum_{i} c'_{i} \delta D_{i}^{2})} +$$

$$\frac{\sqrt{(B + \sum_{i} b_{i} \delta D_{i} + \sum_{i} b'_{i} \delta D_{i}^{2})^{2} - 4(\sum_{i} a_{i} \delta D_{i} + \sum_{i} a'_{i} \delta D_{i}^{2})(C + \sum_{j} c_{j} \delta D_{j} + \sum_{j} c'_{j} \delta D_{j}^{2})}}{2(C + \sum_{i} c_{i} \delta D_{i} + \sum_{i} c'_{i} \delta D_{i}^{2})}$$
(A4)

where we only keep the solution consistent with  $\delta p$  being small. Assuming  $|\delta D_i| \ll M_{i0}$ , both the square root and the reciprical terms can be expanded as a power series in  $\delta D_i$ . Writing only terms up to second order, we obtain:

$$\delta p \simeq -\frac{1}{B} \sum_{i} a_{i} \delta D_{i} - \frac{1}{B} \sum_{i} a'_{i} \delta D_{i}^{2} + \sum_{ij} \frac{\delta D_{i} \delta D_{j}}{B^{2}} \left( \frac{1}{2} (b_{i} a_{j} + b_{j} a_{i}) - \frac{C a_{i} a_{j}}{B} \right)$$

$$\Rightarrow < \delta p > \simeq \sum_{i} \frac{M_{i0}}{B^{2}} \left( b_{i} a_{i} - \frac{C a_{i}^{2}}{B} - B a'_{i} \right)$$
(A5)

where  $\langle ... \rangle$  denotes the expectation operator. We have used the distributive nature of the expectation operator and we have used the results  $\langle \delta D_i \rangle \equiv 0$  and  $\langle \delta D_i \delta D_j \rangle \equiv 0$ , if  $i \neq j$  or  $= M_{i0}$  if i = j, which are true for both Poisson and Gaussian distributions (provided the latter has a statistical error in bin i,  $\sigma_i = \sqrt{\langle D_i \rangle}$ ).

In general,  $\langle \delta p \rangle$  will be nonzero. To estimate its magnitude it is helpful to define  $M'_{i0} \equiv M_{i0} f'_i(p_0)/p_0$ ,  $M''_{i0} \equiv M_{i0} f''_i(p_0)/p_0^2$  and  $M_{i0} \equiv N_c m_{i0}$ , where  $N_c$  is the total number of counts in the dataset. Making these substitutions and rearranging we find that

$$b_i a_i = \frac{f_i'}{p_0^3} (f_i'^2 + f_i''), \qquad -\frac{C}{B} a_i^2 = -\frac{3f_i'^2 \overline{f'f''}}{2p_0^3 \overline{f''^2}} \quad \text{and} \quad Ba_i' = -\frac{f_i' \overline{f'^2}}{p_0^3 m_{i0}}$$
(A6)

where  $\overline{f'^2} \equiv \sum_i f_i'^2 m_{i0}$ , i.e. the model-weighted average of  $f_i'^2$ , and so on. We note that

$$\frac{M_{i0}f_i''}{p_0^2} = M_{i0}'' = \frac{dM_{i0}'}{dp_0} = \frac{M_{i0}}{p_0^2} \left( f_i'^2 - f_i' + p_0 \frac{df_i'}{dp_0} \right) \Rightarrow f_i'' = f_i'^2 - f_i' + p_0 \frac{df_i'}{dp_0}$$
(A7)

and so, on average,  $f_i'f_i'' \sim f_i'^3$  for a broad class of problem, where the  $\sim$  symbol indicates similar orders of magnitude. Thus, on average  $b_ia_i \sim f_i'^3/p_0^3$ ,  $-Ca_i^2/B \sim -f_i'^3/p_0^3$  and  $-Ba_i' \sim -Nf_i'^3/p_0^3$ , where we have used  $1/m_{i0} \sim N$ , the

number of data bins. Since  $N \gg 1$  in general, it follows that the third of the parenthetical terms in Eqn A5 is much larger than the other two. Keeping only that term, Eqn A5 becomes

$$<\delta p>\simeq -\frac{p_0 N}{N_c} \left[ \frac{\sum_i \frac{1}{N} f_i'}{\overline{f'^2}} \right]$$
 (A8)

To estimate  $f_b$ , we adopt the statistical error obtained from fitting the C-statistic, which is expected to be close to that obtained with  $\chi^2$  methods (Cash 1979). As we show in Appendix B, to second order this is given by:

$$<\delta p^{2}>\simeq \frac{\sum_{i}M'_{i0}^{2}M_{i0}}{\left(\sum_{i}M'_{i0}^{2}\right)^{2}} = \frac{p_{0}^{2}}{N_{c}}\frac{\sum_{i}m_{i0}^{3}f'_{i}^{2}}{\left(\sum_{i}m_{i0}^{2}f'_{i}^{2}\right)^{2}} \sim \frac{p_{0}^{2}}{N_{c}\overline{f'^{2}}}$$
 (A9)

We have assumed  $\sum_i m_{i0}^j f_i'^2 \sim \overline{f'^2}/N^{j-1}$ , which is justified since  $m_{i0} \sim 1/N$ . Thus we obtain:

$$f_b \sim -\frac{N}{\sqrt{N_c}} \left[ \frac{\sum_i \frac{1}{N} f_i'}{\sqrt{f'^2}} \right] \sim \mp \frac{N}{\sqrt{N_c}}$$
 (A10)

where we have assumed the term in square brackets is  $\sim \pm 1$ , that is the absolute value of the mean of  $f'_i$  (averaged over the data set) is of the same order of magnitude as its (model-weighted) root mean square. This will likely be approximately true for an arbitrary model (although it should be verified in any particular case) unless one takes considerable care over choosing the particular parameterization of the model, in which case it may be possible to obtain  $f_b$  close to zero.

Strictly speaking, this derivation is only valid for single-parameter models. However, it is relatively straightforward to generalize it to the multi-parameter case, which leads to a set of coupled quadratic equations (one per parameter) of a form similar to Eqn A3. This implies that the bias on the parameters, or at least some combination of the parameters, should be of a similar order to that derived above.

### A2. Model weighting

For the case of model weighting, the problem is remarkably similar. Starting with Eqn 3 differentiating and rearranging, we obtain

$$0 = \frac{d\chi_m^2}{dp} = \sum_i \frac{dM_i}{dp} \left(\frac{M_i^2 - D_i^2}{M_i^2}\right) \tag{A11}$$

Using the same expansion methods we adopted for the data-weighting case, we obtain (ignoring all terms higher than second order):

$$0 \simeq \sum_{i} -\frac{2M'_{i0}}{M_{i0}} \delta D_{i} + \sum_{i} -\frac{M'_{i0}}{M_{i0}^{2}} \delta D_{i}^{2} + \delta p \left[ \sum_{i} \frac{2M'_{i0}^{2}}{M_{i0}} + \sum_{i} \left( \frac{4M'_{i0}^{2}}{M_{i0}^{2}} - \frac{2M''_{i0}}{M_{i0}} \right) \delta D_{i} + \sum_{i} \left( \frac{2M'_{i0}^{2}}{M_{i0}^{3}} - \frac{M''_{i0}}{M_{i0}^{2}} \right) \delta D_{i}^{2} \right] + \delta p^{2} \left[ \sum_{i} \left( \frac{3M'_{i0}M''_{i0}}{M_{i0}} - \frac{3M'_{i0}^{3}}{M_{i0}^{2}} \right) + \sum_{i} \left( -\frac{6M'_{i0}^{3}}{M_{i0}^{3}} + \frac{6M'_{i0}M''_{i0}}{M_{i0}^{2}} - \frac{M''''_{i0}}{M_{i0}} \right) \delta D_{i} + \sum_{i} \left( -\frac{3M'_{i0}}{M_{i0}^{4}} + \frac{3M'_{i0}M''_{i0}}{M_{i0}^{3}} - \frac{M'''_{i0}}{2M_{i0}^{2}} \right) \delta D_{i}^{2} \right]$$
(A12)

which is a quadratic in  $\delta p$ , of the form discussed in the previous section. Therefore, the bias can be trivially computed from Eqn A5. Substituting for  $M_{i0}$ ,  $M'_{i0}$  and  $M''_{i0}$ , exactly as before, we obtain

$$b_i a_i \sim \frac{4f_i'}{p_0^3} \left( f_i'' - 2f_i'^2 \right), \quad -\frac{Ca_i^2}{B} \sim \frac{6f_i'^2}{p_0^3} \left( \frac{\overline{f'^3} - \overline{f'f''}}{\overline{f'^2}} \right) \quad \text{and} \quad -Ba_i' \sim \frac{2f_i'\overline{f'^2}}{m_{i0}p_0^3}$$
(A13)

Following the arguments used for the data-weighting case, it is clear that  $|Ba'_i|$  is much larger than the other terms,

$$<\delta p> \simeq \frac{1}{2} \frac{p_0 N}{N_c} \left[ \frac{\sum_i \frac{1}{N} f_i'}{\overline{f'^2}} \right] \Rightarrow f_b \sim \frac{1}{2} \frac{N}{\sqrt{N_c}} \left[ \frac{\sum_i \frac{1}{N} f_i'}{\sqrt{\overline{f'^2}}} \right] \sim \pm \frac{1}{2} \frac{N}{\sqrt{N_c}}$$
 (A14)

Note that the bias due on parameters recovered under the  $\chi_d^2$  approximation is -2 times the bias with  $\chi_m^2$ .

### B. CASH C-STATISTIC BIAS AND ERROR

We here estimate the magnitude of the bias and the statistical error we expect on the recovered parameter for the case where the Cash C-statistic is used to fit the data. In general, it is expected that parameters obtained from a maximum likelihood method have some level of bias (e.g. Ferguson 1982) but we here show that, for the C-statistic in the high counts regime, this bias is likely far smaller than the statistical error. We can approach this problem by essentially the same technique used in Appendix A. Differentiating Eq 1, setting it equal to 0 and rearranging, we obtain:

$$0 = \sum_{i} \frac{dM_i}{dp} \left( \frac{M_i - D_i}{M_i} \right) \tag{B1}$$

Using the expansion methods we adopted in Appendix A, we obtain the approximate expression:

$$0 = -\sum_{i} M'_{i0} \delta D_{i} + \delta p \left[ \sum_{i} M'_{i0}^{2} + \sum_{i} \left( -M''_{i0} + \frac{M'_{i0}^{2}}{M_{i0}} \right) \delta D_{i} \right]$$

$$+ \delta p^{2} \left[ \left( \sum_{i} \frac{3}{2} M''_{io} M'_{io} - \frac{M'^{3}_{i0}}{M_{i0}} \right) + \sum_{i} \left( -\frac{M'''_{i0}}{2} + \frac{M'_{i0} M''_{i0}}{2M_{i0}} - \frac{M'^{3}_{i0}}{M^{2}_{i0}} \right) \delta D_{i} \right] + \dots$$
(B2)

If higher order terms can be ignored, this is just a quadratic equation similar to that solved in Appendix A, but with  $a'_i = b'_i = c'_i = 0$ . From Eqn A5 it is easy to show that only keeping terms up to second order,

$$<\delta p^2> \simeq \frac{1}{B^2} \sum_{ij} a_i a_j < \delta D_i \delta D_j> = \frac{1}{B^2} \sum_i a_i^2 M_{i0} = \frac{\sum_i M_{i0}^{\prime 2} M_{i0}}{\left(\sum_i M_{i0}^{\prime 2}\right)^2}$$
 (B3)

Now, in general the C-statistic fits are found to be far less biased than those using  $\chi_d^2$  or  $\chi_m^2$ . This can be shown by substituting the appropriate expressions for each of the terms in Eqn A5 and making the various substitutions for  $M_{i0}$ ,  $M'_{i0}$  and  $M''_{i0}$  outlined in Appendix A. We obtain:

$$<\delta p> \simeq \frac{p_0}{N_c} \left[ \frac{\sum_{j} m_{j0}^2 f_j'^2 \sum_{i} \left( m_{i0}^3 f_i' f_i'' - f_i'^3 m_{i0}^3 \right) - \sum_{j} m_{j0}^3 f_j'^2 \sum_{i} \left( \frac{3}{2} m_{i0}^2 f_i' f_i'' - f_i'^3 m_{i0}^2 \right)}{\left( \sum_{j} m_{j0}^2 f_j'^2 \right)^3} \right]$$
(B4)

Now, assuming  $\sum_i m_{i0}^k f_i'^2 \sim \overline{f'^2}/N^{k-1}$  (see Appendix A), we obtain:

$$<\delta p> \sim \frac{p_0}{N_c} \left[ -\frac{\overline{f'f''}}{2\left(\overline{f'^2}\right)^2} \right]$$
 (B5)

where we have allowed two terms of order  $\overline{f'^3}$  in the numerator of the bracketed expression to cancel; although they are unlikely to cancel completely we assume that they largely do so, making the  $\overline{f'f''}$  term more important. Relaxing this assumption does not affect our conclusions. Adopting the order of magnitude estimate for the statistical error derived in Appendix A, we obtain

$$f_b \sim \frac{1}{\sqrt{N_c}} \left[ -\frac{\overline{f'f''}}{2\left(\overline{f'^2}\right)^{\frac{3}{2}}} \right] \sim \mp \frac{1}{\sqrt{N_c}}$$
 (B6)

which is vanishingly small as  $N_c$  becomes large. We have assumed that the term in square brackets is of order unity. This can be justified because, as shown in Appendix A,  $\overline{f'f''} \sim \overline{f'^3}$  which  $\sim (\overline{f'^2})^{3/2}$  for a broad range of problem. Although the accuracy of this assumption should be tested for any given problem, provided  $\overline{f'f''}$  is not larger than  $(\overline{f'^2})^{3/2}$  by a factor  $\sim N(\gg 1)$ , the parameters recovered from the C-statistic fit will be less biased than those using  $\chi_d^2$  or  $\chi_m^2$ . Finally, since typically  $f_b \ll 1$  we are justified in assuming  $\sqrt{<\delta p^2>}$  is the 1- $\sigma$  statistical error on p.

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